

Chloromethane
74-87-3 | DTXSID0021541

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.04e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.78e-01

Confidence level: 5.60e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chloromethane</div> <div>Measured: 1.05e-01</div> <div>Predicted: 5.04e-02</div>	<div>Image not found</div> <div>Chloroethane</div> <div>Measured: 8.80e-02</div> <div>Predicted: 8.70e-02</div>	<div>Image not found</div> <div>Dichloromethane</div> <div>Measured: 1.53e-01</div> <div>Predicted: 1.22e-01</div>
<div>Image not found</div> <div>Ethylene</div> <div>Measured: 4.67e-03</div> <div>Predicted: 7.89e-03</div>	<div>Image not found</div> <div>Methane</div> <div>Measured: 1.37e-03</div> <div>Predicted: 7.88e-03</div>	